

Density instabilities in a two-dimensional dipolar Fermi gas

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We study the density instabilities of a two-dimensional gas of dipolar fermions with aligned dipole moments. The Random Phase Approximation (RPA) for the density-density response function is never accurate for the dipolar gas, and so we incorporate correlations beyond RPA via an improved version of the Singwi-Tosi-Land-Sjölander scheme. In addition to density-wave instabilities, our formalism captures the collapse instability that is expected from Hartree-Fock calculations but is absent from RPA. Crucially, we find that when the dipoles are perpendicular to the layer, the system spontaneously breaks rotational symmetry and forms a stripe phase, in defiance of conventional wisdom.

Ultracold atomic gases have thus far provided a veritable playground in which to explore quantum many-body phenomena. One of the field's great successes is the ability to tune the effective interatomic interactions via Feshbach resonances, thus allowing one to access the regime of strong correlations in a controllable manner. Furthermore, the ability to create tightly bound heteronuclear Feshbach molecules with a permanent electric dipole moment provides a promising system in which to study many-body physics with long-ranged dipole-dipole interactions (for a review see, e.g., Ref. [1]). Indeed, such polar molecules can have interactions that are several orders of magnitude larger than those for atomic magnetic dipoles [2].

Of particular interest are fermionic polar molecules confined in two-dimensional (2D) geometries: fermionic ⁴⁰K⁸⁷Rb molecules have been very recently created [3], cooled down to quantum degeneracy [4], and their lifetime increased by the confinement in 2D [5]. However, correlations are expected to be enhanced in 2D compared to 3D, and thus a major challenge is how to describe theoretically such correlations in the dipolar system. It is this issue that we will address in this Letter.

We focus on a dipolar Fermi gas in a *single* layer, where the dipole moments are all aligned by an external electric field \mathbf{E} , making an angle θ with respect to the normal of the 2D $x - y$ plane (inset of Fig. 1). Even for this simple 2D geometry, the anisotropic interactions provide an exotic twist to the problem and a rich phase diagram is expected. For sufficiently large tilting angles, $\theta > \arcsin(1/\sqrt{3})$, the interaction develops an attractive sliver in the plane, eventually leading to p -wave superfluidity [6]. For small tilting angles $\theta \neq 0$, the repulsive, anisotropic interaction is expected to give rise to anisotropic density-wave (stripe) phases [7, 8], before eventually yielding a Wigner crystal at sufficiently high densities and/or strong interactions [9]. However, in Refs. [7, 8], the basic description of the stripe phase is derived from the Random Phase Approximation (RPA)

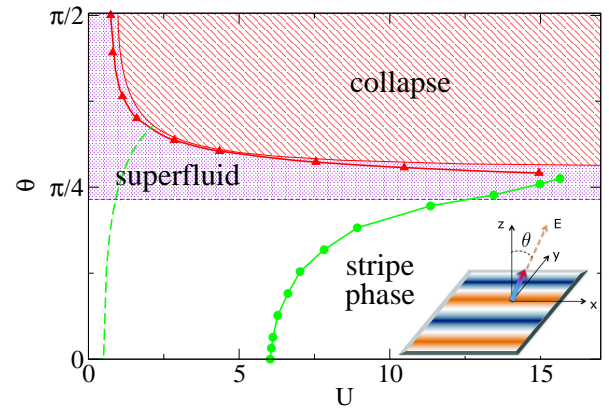


FIG. 1: (Color online) Phase diagram for a 2D dipolar Fermi gas as a function of the dipole orientation angle θ , as defined in the inset, and dimensionless interaction strength $U = mD^2k_F/\hbar^2$, where D is the dipole moment and k_F is the Fermi wave vector. The (green) circles mark the transition to a stripe phase while the (red) triangles correspond to the collapse instability, all derived using our improved STLS formalism. For comparison, we include the RPA result for the stripe instability (dashed [green] line), the Hartree-Fock result for the collapse instability (stripe pattern [red] region), and the area where p -wave superfluidity is expected to occur (shaded [violet] region), as predicted by Ref. [6].

for the density-density response function, and this is not expected to be accurate for the 2D dipolar Fermi gas: As well as neglecting the exchange correlations resulting from Fermi statistics, RPA fails to correctly describe the long wavelength regime of the density-density response function, unlike in the case of the 2D electron gas. Furthermore, RPA does not settle the question of whether or not the 2D dipolar Fermi gas spontaneously breaks rotational symmetry and forms a stripe phase for *isotropic* interactions ($\theta = 0$), which is of fundamental interest to other quasi-2D systems such as the cuprate superconductors [10].

In this Letter, we include correlations beyond RPA

using an improved version of the Singwi-Tosi-Land-Sjölander (STLS) scheme [11], which has had much success in describing electron systems [12]. Using this formalism, the effect of correlations is evident in the pair correlation function, where we observe a “correlation hole” forming around each fermion with increasing interaction. We map out the instabilities of the density-density response function and we see the existence of a stripe phase, similarly to RPA, though for considerably larger dipole strengths and/or densities. However, in contrast to RPA, we also observe a collapse instability for sufficiently large θ , which is consistent with Hartree-Fock calculations [6, 8, 13, 14]. Last but not least, we show that the system does indeed spontaneously break rotational symmetry to form a stripe phase when $\theta = 0$.

The effective 2D dipolar interaction for aligned dipoles confined in a layer of width W can be evaluated as per Ref. [15]. Parametrizing the x - y in-plane momentum in polar coordinates $\mathbf{q} = (q, \phi)$ ($\phi = 0$ corresponds to the direction x of the dipole tilt in the inset of Fig. 1), in the limit $qW \ll 1$ (the expected regime of the experiments), the 2D interaction can be written as:

$$v(q, \phi) = V_0 - 2\pi D^2 q (\cos^2 \theta - \sin^2 \theta \cos^2 \phi) , \quad (1)$$

where D is the dipole moment. V_0 corresponds to the short-ranged contact interaction, which depends on the confinement, and the confinement width W provides a natural cut-off for the quasi-2D system: $\Lambda \sim 1/W \gg k_F$. The dipolar system is parametrized by the angle θ and the dimensionless interaction strength $U = mD^2 k_F / \hbar^2$, where m is the fermion mass and $k_F = \sqrt{4\pi n}$ is the Fermi wave vector (n is the density). Note that the effective coupling increases with increasing density, in contrast to the case of Coulomb interactions, where the regime of strong coupling corresponds to low densities.

In the following, we analyse the inhomogeneous phases of a 2D dipolar Fermi gas using the linear response theory. Here, the linear density response $\delta n(\mathbf{q}, \omega)$ to an external perturbing potential $V^{ext}(\mathbf{q}, \omega)$ defines the density-density response function $\chi(\mathbf{q}, \omega)$ in frequency and momentum space:

$$\delta n(\mathbf{q}, \omega) = \chi(\mathbf{q}, \omega) V^{ext}(\mathbf{q}, \omega) . \quad (2)$$

In the static limit, $\omega = 0$, the appearance of a divergence in χ at a particular wave vector \mathbf{q}_c signals an instability towards the formation of a density wave with period set by \mathbf{q}_c . Note that if the instability only depends on the magnitude $q_c \equiv |\mathbf{q}_c|$ and is insensitive to the angle ϕ , then the inhomogeneous phase may consist of multiple density waves, so that it forms, e.g., a triangular lattice rather than a stripe phase.

In addition to density instabilities, we can use the fluctuation-dissipation theorem to extract the ground-state correlation functions from $\chi(\mathbf{q}, \omega)$. A standard quantity is the pair correlation function $g(\mathbf{r}_2 - \mathbf{r}_1) =$

$\frac{1}{n^2} \langle \psi^\dagger(\mathbf{r}_2) \psi^\dagger(\mathbf{r}_1) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2) \rangle$, where $\langle \dots \rangle$ is the expectation over the ground state and $\psi^\dagger(\mathbf{r})$ is the creation operator for a spinless fermion at position \mathbf{r} . This is related to the static structure factor $S(\mathbf{q})$ by:

$$g(\mathbf{r}) = 1 + \frac{1}{n} \int \frac{d\mathbf{q}}{(2\pi)^2} e^{i\mathbf{q} \cdot \mathbf{r}} [S(\mathbf{q}) - 1] . \quad (3)$$

which, in turn, is connected to the response function via

$$S(\mathbf{q}) = -\frac{\hbar}{n\pi} \int_0^\infty d\omega \chi(\mathbf{q}, i\omega) . \quad (4)$$

Note that here the integration is performed along the imaginary frequency axis.

For a non-interacting 2D Fermi gas at zero temperature, the response function can be evaluated exactly [16],

$$\Pi(\mathbf{q}, i\omega) = \frac{m}{2\pi b} \left\{ \sqrt{2} \left[a + \sqrt{a^2 + (\omega b)^2} \right]^{1/2} - b \right\} ,$$

with $a = \frac{b^2}{4} - b \frac{k_F^2}{m} - \omega^2$ and $b = \frac{q^2}{m}$. If we insert $\Pi(\mathbf{q}, i\omega)$ into (4) to obtain the non-interacting structure factor $S_0(\mathbf{q})$, and then use Eq. (3), we find that $g(0) = 0$ (see Fig. 3), as expected from Pauli exclusion.

For fermions interacting via a two-body potential $v(\mathbf{q})$, one often relies [7, 8] upon the RPA to estimate χ . Here, the response is that of a non-interacting system, $\Pi(\mathbf{q}, \omega)$, to an external potential which includes an effective potential due to the perturbed density, i.e., one replaces $V^{ext}(\mathbf{q}, \omega)$ in (2) with $V^{ext}(\mathbf{q}, \omega) + v(\mathbf{q})\delta n(\mathbf{q}, \omega)$, giving $\chi_{RPA}^{-1}(\mathbf{q}, \omega) = \Pi^{-1}(\mathbf{q}, \omega) - v(\mathbf{q})$. However, as discussed below, RPA is never accurate for dipolar interactions.

We account for correlations beyond RPA by including a local field factor $G(\mathbf{q})$ in the response function [12]:

$$\chi(\mathbf{q}, \omega) = \frac{\Pi(\mathbf{q}, \omega)}{1 - v(\mathbf{q}) [1 - G(\mathbf{q})] \Pi(\mathbf{q}, \omega)} . \quad (5)$$

Physically, $G(\mathbf{q})$ corresponds to the corrections to the RPA effective potential that stem from correlations between fermions. For example, at short distances (large q) the interactions will be suppressed by Pauli exclusion, thus giving $G = 1$. These exchange correlations, which are crucial in a gas of identical fermions, are clearly neglected by RPA. In addition, we can also extract the behavior of G in the opposite limit $q \rightarrow 0$ using the compressibility sum rule [12, 17], which relates $\chi^{-1}(\mathbf{q} \rightarrow 0, 0)$ to the inverse compressibility $\kappa^{-1} = n^2 \partial^2(n\varepsilon) / \partial n^2$, where ε is the ground state energy per particle. For Coulomb interactions in electron systems, where $v(\mathbf{q}) \propto 1/q$, the Hartree-Fock calculation for ε gives us $G(\mathbf{q}) \simeq 10q/(3\pi k_F)$ as $q \rightarrow 0$, thus confirming that $G \rightarrow 0$: RPA is therefore a reasonable approximation for long wavelengths [12]. This is not however true in the case of dipolar interactions: If we perform the same procedure, where we take $\theta = 0$ in Eq. (1) for simplicity,

then we find that $G(0) = 1 - 32\hbar^2 U / (3mV_0)$ in the limit $U \ll 1$, where the Hartree-Fock result (7) is valid. Thus we see that χ_{RPA} is never recovered in this case, even in the weak-coupling limit. In sum, the RPA for 2D dipolar Fermi gases fails at both short and long wavelengths [25].

We instead determine $G(\mathbf{q})$ using the STLS scheme, which provides an ingenious way in which to feed back the correlations in $\chi(\mathbf{q}, \omega)$ into $G(\mathbf{q})$. STLS uses a classical analogy for the system's response to obtain [11]

$$G(\mathbf{q}) = -\frac{1}{n} \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{\mathbf{q} \cdot \mathbf{k}}{q^2} \frac{v(\mathbf{k})}{v(\mathbf{q})} [S(\mathbf{q} - \mathbf{k}) - 1]. \quad (6)$$

Note that the RPA case of $G = 0$ implies that $S(\mathbf{q}) = 1$ here, which in turn corresponds to setting $g(\mathbf{r}) = 1$, i.e. neglecting any correlations in the STLS classical analogy. Combining Eq. (6) with Eq. (4) gives us a set of self-consistent equations for $G(\mathbf{q})$ that can be solved iteratively. If we start by inserting $S_0(\mathbf{q})$ into Eq. (6) (which is equivalent to setting $G^{(0)}(\mathbf{q}) = 1$ at the beginning of the iteration), then $G^{(1)}(\mathbf{q})$ incorporates exchange correlations only. In particular, if we have purely contact interactions $v(\mathbf{q}) = V_0$, then Eq. (6) returns $G^{(1)}(\mathbf{q}) = 1 - g(0) = 1$. Thus, we see that STLS correctly gives us a non-interacting response for a gas of identical fermions with contact interactions.

For the dipolar interaction (1), one can show that $G(\mathbf{q})$ calculated from Eq. (6) will also render $\chi(\mathbf{q}, \omega)$ independent of V_0 provided $g(0) = 0$. However, similarly to what happens in the electronic Coulomb case [12], the STLS scheme does not guarantee that $g(0) = 0$ for the converged solution and so we obtain an unphysical dependence on V_0 . In addition, we find that the density instabilities determined using this procedure are sensitive to the cut-off Λ at large q even though we have $q_c \leq 2k_F$.

To address these issues and better model the dipolar gas, we improve the STLS scheme by imposing, at each iteration step, the constraint $g(0) = 0$ and the fact that $\chi(\mathbf{q}, \omega)$, and thus $S(\mathbf{q})$, will be dominated by Pauli exclusion for $q \gg 2k_F$. Similarly to Ref. [18], we achieve this by adding a corrective function $\delta S(\mathbf{q})$ to the $S(\mathbf{q})$ defined by Eq. (4) and then using $S + \delta S$ to determine $G(\mathbf{q})$. In particular, we use the ansatz

$$\delta S(\mathbf{q}) = \left(S_0(\mathbf{q}) - S(\mathbf{q}) + A e^{-q^2/(2k_F)^2} \right) \left(1 - e^{-q^2/(2k_F)^2} \right)$$

to interpolate between the STLS result for $q < 2k_F$ and the non-interacting one S_0 for $q \gg 2k_F$, where exchange correlations dominate. The constant A adjusts the behavior near $q = 2k_F$ and is chosen at each iteration step so that $g(0) = 0$. Note that the correction around $q \simeq 2k_F$ is generally small. Our improved STLS procedure thus renders $\chi(\mathbf{q}, \omega)$ insensitive to both V_0 and cut-off $\Lambda \gg 2k_F$, as required.

We have confirmed that our converged solution for $U \ll 1$ agrees with the weak-coupling Hartree-Fock result. In this limit, the Hartree-Fock approximation for

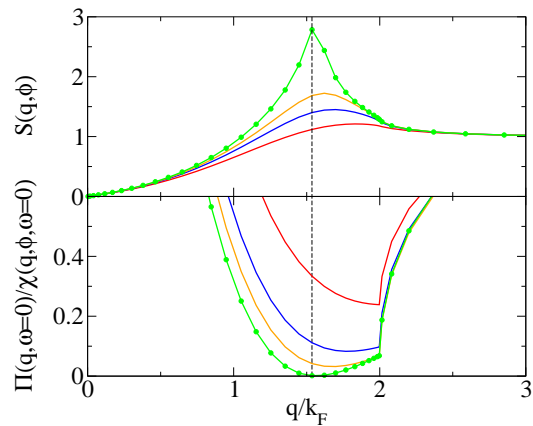


FIG. 2: (Color online) Behaviour of the static structure factor $S(q, \phi)$ and the rescaled inverse density-density response function, $\Pi(q, \omega = 0)/\chi(q, \phi; \omega = 0)$, as the stripe instability at $\phi = \pi/2$ is approached for $\theta = 0.1$. The vertical dashed line marks the position of the unstable wave vector $q_c \simeq 1.54k_F$.

the dipolar gas gives us a ground-state energy per particle:

$$\varepsilon_{HF} = \frac{\hbar^2 k_F^2}{m} \left[\frac{1}{4} + \frac{16}{45\pi} U (3 \cos^2 \theta - 1) \right]. \quad (7)$$

Here, we only consider up to first-order in U for the energy density ε_{HF} , and thus we have neglected the higher order terms due to Fermi surface deformations induced when $\theta \neq 0$ [8]. We compare this expression with the ground state energy density extracted from our STLS solution for $\chi(\mathbf{q}, \omega)$ using the following relation for the interaction energy per particle:

$$\varepsilon_{int} = \frac{n}{2} v(0) + \frac{1}{2} \int \frac{d\mathbf{q}}{(2\pi)^2} v(\mathbf{q}) [S(\mathbf{q}) - 1] \quad (8)$$

and then employing the Hellman-Feynman theorem [12, 17]. By doing this, we find that the ground state energy density obtained via the STLS calculation recovers the Hartree-Fock result (7) when $U \ll 1$. Equivalently, we recover ε_{HF} if we impose $S(\mathbf{q}) = S_0(\mathbf{q})$ in Eq. (8).

Using our procedure, we analyse the density instabilities of the converged solutions for $\chi(\mathbf{q}, \omega)$. For tilted dipoles ($\theta \neq 0$), $\chi(\mathbf{q}, 0)$ is most unstable towards forming a density wave along $\phi = \pi/2$, as shown in the Fig. 1 inset. Referring to the phase diagram in Fig. 1, we find that this stripe phase exists for sufficiently large U when $\theta \lesssim \pi/4$. RPA also predicts a stripe transition for $1/U = 2 \cos^2 \theta$ once one sets $V_0 = 0$ in Eq. (1) (cf. Refs. [7, 8]). However, we see that correlations shift the transition to a much higher U compared to the RPA result, thus giving p -wave superfluidity [6] a sizeable region of existence around $\theta = \pi/4$. Moreover, we find that $q_c < 2k_F$ rather than $q_c = 2k_F$ as expected from RPA. Figure 2 shows how $\chi(\mathbf{q}, 0)^{-1}$ tends toward zero (i.e. how $\chi(\mathbf{q}, 0)$ diverges) as we approach the stripe transition at

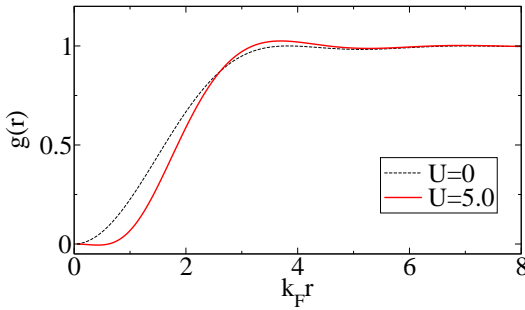


FIG. 3: (Color online) Pair correlation function $g(r)$ of a 2D dipolar Fermi gas at $\theta = 0$ with and without interactions. Note that we must always have $g(0) = 0$ for a gas of identical fermions. Increasing the repulsive interaction U decreases the likelihood of two fermions being close together, thus resulting in a “correlation hole” near $r = 0$ for $U > 1$.

fixed θ . The divergence in $\chi(\mathbf{q}, 0)$ leads to a singularity in Eq. (4), thus yielding a corresponding peak in the structure factor $S(q, \phi)$ at $q = q_c$. Once $\chi(\mathbf{q}, 0)^{-1}$ hits zero at the stripe transition, we find that we no longer obtain convergence of the self-consistent equations (4) and (6) when we increase U further.

For the isotropic case ($\theta = 0$), one might expect the inhomogeneous phase to maximise its rotational symmetry by forming a triangular lattice. However, we instead find that the system spontaneously breaks rotational symmetry to form a stripe phase. We see this by setting $G^{(0)}(\mathbf{q})$ to a converged solution for small θ and U , and then examining whether or not the iteration procedure for $\theta = 0$ amplifies or suppresses the spread in ϕ . From the final converged solutions, we find that $\chi(\mathbf{q}, 0)$ exhibits a large spread in ϕ at $U = 6$, before eventually diverging for a specific ϕ at $U \simeq 6.03$. Here, the direction of the stripe is simply determined by the original ϕ dependence of $G^{(0)}(\mathbf{q})$. Thus, we see that the system is unstable towards breaking rotational symmetry and spontaneously forming a stripe phase [26]. There is also the possibility that the system first forms a nematic phase, similar to that discussed in Ref. [19], before forming a stripe phase.

If we neglect any dependence on ϕ and consider G and S to be functions of q only, then we never see a transition to an inhomogeneous phase. However, we do see evidence of strong correlations in the pair correlation function (Fig. 3) and a peak in the structure factor that suggests an imminent transition. Such a behavior is consistent with a first-order transition to a Wigner crystal phase. If this transition is similar to that of dipolar bosons, then it is expected to occur at $U \simeq 60$ [20–22].

As θ increases towards $\pi/2$ in Fig. 1, we instead find that the system can be unstable towards collapse, where $q_c = 0$ at the instability. In this case, $\chi(\mathbf{q}, 0)$ is most unstable for $\phi = 0$, which implies that the system executes an anisotropic collapse in the direction of the dipole tilt, a physically reasonable scenario. Contrast this with

RPA, where one only ever has $q_c > 0$. Sun et al. [7] use a perturbative expansion of $\chi(\mathbf{q}, 0)$ around $\mathbf{q} = 0$ to argue that one never has instabilities with $q_c = 0$ in the 2D dipolar gas. However, their argument rests on the assumption that $\chi(\mathbf{q}, 0)$ is analytic at $\mathbf{q} = 0$, as is the case with RPA, while we find that our $\chi(\mathbf{q}, 0)$ depends on ϕ at $\mathbf{q} = 0$ and is thus non-analytic. This non-analytic behavior at $\mathbf{q} = 0$ may, at first sight, appear surprising for a Fermi liquid, but it merely corresponds to an anisotropic compressibility, which is physically reasonable for anisotropic interactions. Moreover, it is consistent with the collapse predicted from Hartree-Fock calculations [6, 8, 13, 14], as depicted in Fig. 1. We recover the Hartree-Fock calculations for the collapse by using in Eq. (5) the exchange-only field factor $G^{(1)}(\mathbf{q})$ previously discussed. The Hartree-Fock approximation should be accurate for the collapse instability since the instability simply corresponds to the point at which the attractive interaction exceeds the effective repulsive interaction derived from Pauli exclusion. However, we do not expect such an approximation to be accurate for the stripe instability since we require correlations beyond the exchange ones in this case. Indeed, the conserving Hartree-Fock calculation employed in Refs. [13, 14] is expected to underestimate the interaction at which the stripe transition occurs, as stressed in Ref. [13]. This explains the quantitative disagreement between our phase boundary and that of Refs. [13, 14].

Despite the apparent success of our improved STLS scheme for the dipolar gas, there are still some inconsistencies that it shares with the original STLS scheme for electron systems. Specifically, the pair correlation function can become slightly negative at short distances (Fig. 3) and the compressibility sum rule is systematically violated for a range of interaction strengths $U \lesssim 3$. However, our scheme is a substantial improvement over RPA and we expect it to provide a basis upon which to investigate correlations in other dipolar Fermi systems such as multilayers.

Our predicted stripe phases should be experimentally realizable with polar molecules, where the density modulations could be probed using Bragg scattering. The typical density of polar molecules in a 2D layer is 10^8 cm^{-2} , which gives a maximum of $U \simeq 0.3$ for KRb molecules with dipole moment $D \sim 0.2$ Debye as in the experiment [5]. Thus, to access the stripe phase with current experiments, one needs to enhance U by, e.g., increasing the effective mass using an in-plane optical lattice. Alternatively, one could use LiCs molecules which have a dipole moment of up to 5.5 Debye [23], thus allowing one to explore the stripe transition for the whole range of θ .

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 - [25] Note that, already in Ref. [24] it was recognised that exchange correlations beyond RPA must be incorporated in the dipolar gas. However, they consider a phenomenological expression for the local field factor with a form similar to that in Coulomb systems.
 - [26] Note that this implicitly assumes that the stripe transition is second order, but it could instead be preempted by a first order transition — one needs to consider higher order terms in δn in the free energy to ascertain this.